

Universal property of the information entropy in fermionic and bosonic systems.

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Abstract

It is shown that a similar functional form $S = a + b \ln N$ holds approximately for the information entropy S as function of the number of particles N for atoms, nuclei and atomic clusters (fermionic systems) and correlated boson-atoms in a trap (bosonic systems). It is also seen that rigorous inequalities previously found to hold between S and the kinetic energy T for fermionic systems, hold for bosonic systems as well. It is found that Landsberg's order parameter Ω is an increasing function of N for the above systems. It is conjectured that the above properties are universal i.e. they do not depend on the kind of constituent particles (fermions or correlated bosons) and the size of the system.

Shannon's information entropy for a continuous probability distribution $p(x)$ is defined as

$$S = - \int p(x) \ln p(x) dx \quad (1)$$

where $\int p(x) dx = 1$. S is measured in bits if the base of the logarithm is 2 and nats (natural units of information) if the logarithm is natural.

This quantity is useful for the study of quantum systems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11] and appears in various areas: information theory, ergodic theory and statistical mechanics. It is closely related to the entropy and disorder in thermodynamics. It represents the information content or uncertainty of $p(x)$ and has already been connected with experimental and/or fundamental quantities (e.g. the kinetic energy and magnetic susceptibility in atomic physics [5, 6] and the kinetic energy and mean square radius in nuclear and cluster physics [4]).

In recent years information-theoretic methods play an increasing role for the study of quantum mechanical systems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. An important step was the discovery of an entropic uncertainty relation (EUR)[2], which for a three-dimensional system has the form

$$S = S_r + S_k \geq 3(1 + \ln \pi) \simeq 6.434 \quad (\hbar = 1) \quad (2)$$

where S_r is the information entropy in position space of the density distribution $\rho(\mathbf{r})$ of a quantum system

$$S_r = - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} \quad (3)$$

and S_k is the information entropy in momentum space of the corresponding momentum distribution $n(\mathbf{k})$

$$S_k = - \int n(\mathbf{k}) \ln n(\mathbf{k}) d\mathbf{k} \quad (4)$$

The density distributions $\rho(\mathbf{r})$ and $n(\mathbf{k})$ are normalized to one. It is noted that the entropy sum S does not depend on the units in measuring r and k , i.e. it is scale invariant to a uniform change of coordinates. Inequality (2) provides a lower bound for $S_r + S_k$, which is attained by Gaussian density distributions. Its physical meaning is obvious: an increase of S_k is accompanied by a decrease of S_r and vice versa, which indicates that a diffuse $n(\mathbf{k})$ is associated with a localised $\rho(\mathbf{r})$ and vice versa. This is also expected from the Heisenberg uncertainty relation, but (2) is a strengthened version of the uncertainty principle.

The present Letter addresses the problem of finding S_r , S_k (i.e. the extent of $\rho(\mathbf{r})$ and $n(\mathbf{k})$) for bosonic many-body systems in order to compare with corresponding results for fermionic systems. First, we review previous work for systems of fermions.

In [3] we proposed a universal property for S for the density distributions of nucleons in nuclei, electrons in atoms and valence electrons in atomic clusters. This property has the form

$$S = a + b \ln N \quad (5)$$

where the parameters a , b depend on the system under consideration. The values of the parameters are the following

$$\begin{aligned} a = 5.325 \quad b = 0.858 \quad & \text{(nuclei)} \\ a = 5.891 \quad b = 0.849 \quad & \text{(atomic clusters)} \\ a = 6.257 \quad b = 1.007 \quad & \text{(atoms)} \end{aligned} \quad (6)$$

For the total densities, there is in atomic physics a connection of S_r , S_k with the total kinetic energy T and mean square radius of the system through rigorous inequalities derived using the EUR [6]

$$S_r(\min) \leq S_r \leq S_r(\max) \quad (7)$$

$$S_k(\min) \leq S_k \leq S_k(\max) \quad (8)$$

$$S(\min) \leq S \leq S(\max) \quad (9)$$

The lower and upper limits are written here more conveniently in the following form, for density distributions normalized to one:

$$\begin{aligned} S_r(\min) &= \frac{3}{2}(1 + \ln \pi) - \frac{3}{2} \ln \left(\frac{4}{3} T \right) \\ S_r(\max) &= \frac{3}{2}(1 + \ln \pi) + \frac{3}{2} \ln \left(\frac{2}{3} \langle r^2 \rangle \right) \end{aligned} \quad (10)$$

$$\begin{aligned} S_k(\min) &= \frac{3}{2}(1 + \ln \pi) - \frac{3}{2} \ln \left(\frac{2}{3} \langle r^2 \rangle \right) \\ S_k(\max) &= \frac{3}{2}(1 + \ln \pi) + \frac{3}{2} \ln \left(\frac{4}{3} T \right) \end{aligned} \quad (11)$$

$$\begin{aligned} S(\min) &= 3(1 + \ln \pi) \\ S(\max) &= 3(1 + \ln \pi) + \frac{3}{2} \ln \left(\frac{8}{9} \langle r^2 \rangle T \right) \end{aligned} \quad (12)$$

In a previous Letter [4] we verified numerically that the above inequalities hold for nuclear density distributions and valence electron distributions in atomic clusters. We also found a link of S with the total kinetic energy of the system T , and a relationship of Shannon's information entropy in position-space S_r with an experimental quantity i.e. the rms radius of nuclei and clusters. In Ref [8] we used another definition of entropy according to phase-space considerations [7]. Thus we derived an information-theoretic criterion of the quality of a nuclear density distribution i.e. the larger S , the better the quality of the nuclear model. Another interesting result [13] is the fact that the entropy of an N -photon state subjected to Gaussian noise increases linearly with the logarithm of N . In Ref. [10] we considered the single-particle states of a nucleon in nuclei, a Λ in hypernuclei and a valence electron in atomic clusters. We proposed a connection of S with the energy E of single-particles states through the relation

$$S = k \ln(\mu E + \nu) \quad (13)$$

where k , μ and ν depend on the system. It is interesting that the same relation holds for various systems.

In the present Letter we verify numerically that inequalities (7), (8) and (9) hold for a correlated bosonic system as well, i.e. trapped boson-alkali atoms [14, 15, 16] as shown in Table 1. It is noted that for large N S_k may become negative, but the important quantity is the net information content $S = S_r + S_k$ of the system which is positive. We employed density distributions $\rho(\mathbf{r})$ and $n(\mathbf{k})$ for bosons derived by solving numerically the Gross-Pitaevskii equation of the form

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega^2 r^2 + N \frac{4\pi \hbar^2 a}{m} |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}), \quad (14)$$

where N is the number of the atoms, a is the scattering length of the interaction and μ is the chemical potential [15].

For a system of non-interacting bosons in an isotropic harmonic trap the condensate has a Gaussian form of average width b ($b = (\hbar/m\omega)^{1/2}$). If the atoms are interacting, the shape of the condensate can be changed significantly with respect to the Gaussian. The ground-state properties of the condensate for weakly interacting atoms are explained quite successfully by the non-linear equation (14).

We solved numerically this equation for trapped boson-alkali atoms (^{87}Rb) systems with parameter $b = 12180 \text{ \AA}$ (angular frequency $\omega/\pi = 77.78 \text{ Hz}$) and scattering length $a = 52.9 \text{ \AA}$. In this case the effective atomic size is small compared both to the trap size and to the interatomic distance ensuring the diluteness of the gas. The density distribution $\rho(\mathbf{r})$, obtained in this way, and the momentum distribution $n(\mathbf{k})$, obtained by taking the Fourier transform of the ground-state wave function $\psi(\mathbf{r})$, were inserted into equations (3) and (4) to find the values of S_r , S_k and $S = S_r + S_k$ as functions of the number of bosons N . The results are shown in Fig. 1. The circles correspond to our calculated values, while the line to our fitted form

$$S = S_r + S_k = a + b \ln N$$

where $a = 6.033$, $b = 0.068$ and $5 \times 10^2 < N < 10^6$.

It is noted that the validity of (14) is based on the condition that the s-wave scattering length be much smaller than the average distance between atoms and that the number of atoms in the condensate be much larger than one [15].

It is seen that a similar functional form holds approximately for S as function of the number of particles N for fermionic and bosonic systems (correlated atoms in a trap).

Landsberg [12] defined the order parameter Ω as

$$\Omega = 1 - \Delta = 1 - \frac{S}{S(\max)} \quad (15)$$

where S is the information entropy (actual) of the system and $S(\max)$ the maximum entropy accessible to the system. Thus the concepts of entropy and disorder are decoupled and it is possible for the entropy and order to increase simultaneously. It is noted that $\Omega = 1$ corresponds to perfect order and predictability, while $\Omega = 0$ means complete disorder and randomness.

Our results in the present work for S and $S(\max)$ allows us to calculate Ω as function of the number of particles N in a system of trapped correlated boson-alkali atoms. The dependence $\Omega(N)$ is presented in Figure 2. It is seen that Ω is an increasing function of N . A similar trend has been observed in Fig. 1 of Ref. [11], where $\Omega(N)$ was calculated for nucleons in nuclei and valence electrons in atomic clusters. As stated in [11], our result is in a way counter-intuitive and indicates that as particles are added in a correlated quantum-mechanical system, the system becomes more ordered. The authors in [17] studied disorder and complexity in an ideal Fermi gas of electrons. They observed that for a small number of electrons the order parameter Ω is small, while Ω increases as one pumps electrons into the system and the energy levels fill up.

Concluding, we may state that fermionic and correlated bosonic systems show certain similarities from an information-theoretic point of view. The information entropy S obeys for both the same functional form $S = a + b \ln N$. We have also shown that the same rigorous inequalities (upper and lower limits) hold for both systems. Finally, we have shown that Landsberg's order parameter Ω is an increasing function of the number of particles N for both systems. It is conjectured that the above properties are universal for fermionic and bosonic many-body quantum systems. It is also remarkable that those properties hold for systems of different sizes i.e. ranging from the order of fermis (10^{-13} cm) in nuclei to 10^4 Å (10^{-4} cm) for bosonic systems.

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Table 1: Values of S_r , S_k and S versus the number of particles N for a bosonic system (see inequalities (7), (8) and (9))

N	$S_r(min)$	S_r	$S_r(max)$	$S_k(min)$	S_k	$S_k(max)$	$S(min)$	S	$S(max)$
5×10^2	3.797	3.834	3.845	2.590	2.630	2.637	6.434	6.465	6.482
10^3	4.027	4.100	4.120	2.314	2.394	2.408	6.434	6.494	6.528
3×10^3	4.437	4.599	4.640	1.794	1.963	1.997	6.434	6.562	6.637
5×10^3	4.641	4.855	4.907	1.527	1.746	1.794	6.434	6.601	6.701
7×10^3	4.778	5.029	5.090	1.345	1.598	1.657	6.434	6.627	6.746
10^4	4.925	5.219	5.287	1.148	1.437	1.509	6.434	6.655	6.796
5×10^4	5.615	6.113	6.211	0.223	0.667	0.819	6.434	6.780	7.030
10^5	5.922	6.511	6.619	-0.185	0.317	0.512	6.434	6.828	7.132
5×10^5	6.654	7.452	7.577	-1.142	-0.533	-0.220	6.434	6.919	7.357
10^6	6.993	7.864	7.992	-1.557	-0.920	-0.560	6.434	6.943	7.432

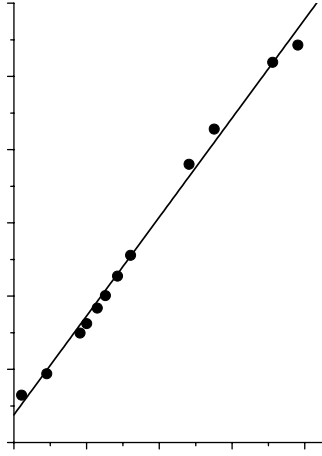


Figure 1: Plot of information entropy $S = S_r + S_k$ as a function of the number of particles N for a bosonic system.

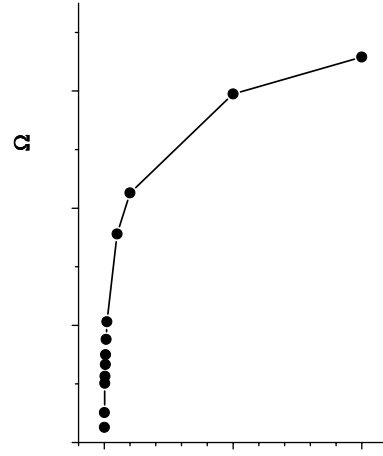


Figure 2: The order parameter Ω as a function of the number of particles N for a bosonic system.